REACTIVE MODELING OF A MTO REACTOR BY COMBINING CRE AND CFD

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Abstract
The methanol to olefins (MTO) process, which is an economical route to produce light olefins from coal resources, has been successfully commercialized in China by DICP (DMTO). Although DMTO process borrows ideas from the modern fluid catalytic cracking (FCC) units, it has unique features in hydrodynamic behaviors for favoring methanol conversion, thus calling for new modeling for scale-up. In addition, the coke content on catalysts greatly affects reaction rate, but its generation is extremely slow. The mean residence time of catalysts hence ranges from minutes to hours for reaching the desired level of coke content. Thus it is a huge challenge for time-dependent computational fluid dynamics (CFD) to simulate this reactive process. To speed up it, the classic chemical reaction engineering (CRE) model is introduced to combine with CFD. Here, the continuous stirred tank reactor (CSTR) model is established to estimate the steady state distribution of coke content as the initial distribution for CFD simulation. Comparison with experimental data shows good agreement and also the great speed-up ratio compared to pure CFD simulation. A series of scale-up simulations are under way.

Keywords
CRE, CFD, Methanol-to-olefins (MTO), EMMS, Fluidized bed.

Introduction
The MTO process, which is an economical route to produce light olefins from coal resources, has been successfully commercialized in China by DICP (Tian et al., 2015). The DMTO units borrow the ideas from the reaction-regeneration design of FCC process. In contrast with FCC, where catalytic cracking reactions are endothermic and prefer a fast fluidization state, the methanol conversion in a DMTO reactor is exothermic and prefers a bubbling or turbulent fluidized bed with longer residence time. The big difference between two designs leaves us much room for optimization. That requires in-depth understanding of the coupling between hydrodynamics and reactions.

The coke content on catalysts is found to be critical on MTO reactions, while its generation is extremely slow. To reach the desired level of coke content, it generally requires minutes or hours to keep the catalysts stay in the reactor. Nowadays, it is not affordable for CFD to carry out such a long simulation. The classic chemical reaction engineering (CRE) models, e.g., plug flow reactor model and continuous stirred tank reactor (CSTR) model, have been widely applied to simplify the coupling between chemical kinetics and hydrodynamics (Levenspiel, 1999). In this study, CSTR model is set up to estimate the steady state distribution of coke content as the initial distribution for CFD simulation. Simulation results of hydrodynamics and product distribution are later presented with comparison to experimental data. Finally, the conclusions and future work are discussed.

Model and settings
The reactor geometry is shown in Fig.1. The Eulerian multiphase granular model in ANSYS Fluent version 15 is employed. The species and energy transport equations are turned on to consider chemical reactions. It has been
recognized that the drag coefficient is greatly affected by inhomogeneous flow structures. Here, EMMS/bubbling model which is calculated by software EMMS®2.0, is chosen. Both gas and solid phase are treated as mixtures, including 9 gas species and 2 solid species, respectively.

CRE-estimated initial distribution

For this operating condition, it requires a run for about one hour to reach the desired level of coke content (~6%). It can be estimated to take 1200 days on our parallel computers (2CPUs per node, Intel-Xeon 2.8G, 10 cores). To speed up it, a CSTR model is established to evaluate the coke content in the bubbling reactor, as shown in Fig.2.

CFD simulation results

Through monitoring the time-evolution of solids inventory, coke content and mass fraction of gaseous product (not shown here), the simulation is found to converge to a stable state after 40 s. The contour of mass fraction of ethylene and propylene are shown in Fig.3. Similar distribution is observed for C₂H₄ and C₃H₆ except the difference in magnitude. That is because the reactions producing C₂H₄ and C₃H₆ are parallel and the mass diffusivity is set as the same for all species in the gas mixture. The MTO reactions mostly take place in the region near the gas distributor below the elevation of 0.2 m, above which the concentration distributions in both axial and radial directions appear to be uniform. Table 1 shows the product predictions of CFD simulation. Besides the mass fraction of gaseous product, the methanol conversion of CFD is much closer to the experiment than the CSTR.

Conclusions and future work

In this study, a CSTR model is combined with CFD to explore the hydrodynamic and reactive behavior of a DMTO reactor, thus greatly shortening the transition time from the initial state to the steady state. The typical behavior of the bubbling fluidized bed under countercurrent flow is captured in our simulations. Great change of mass fractions of light olefins is found near the distributor region. Generally the combination of CFD and CRE brings us better capability for reactive simulation of fluidized beds with long residence time. A series of scale-up simulations ranging from for a small bed to an industrial MTO reactor are under way.

References